MASTER COPY KEEP THIS COPY FOR REPRODUCTION PURPOSES

...UMENTATION PAGE

Form Approved
OMB No. 0704-0188

2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
December 31, 1993	Final

4. TITLE AND SUBTITLE
PERFORMANCE PREDICTIONS FOR COMPOSITE MATERIALS

5. FUNDING NUMBERS
DAAL03-89-K-0144

6. AUTHOR(S)
Professors William M. Gelbart, Shechao Feng, Howard Reiss and Daniel Kivelson

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Departments of Chemistry and Physics
University of California, Los Angeles
Los Angeles, CA 90024

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U. S. Army Research Office
P. O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
ARO 26891.2-MS-A

11. SUPPLEMENTARY NOTES
The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

This project has initiated and brought to completion several novel microscopic approaches to the prediction of material response to applied stress. In a series of several papers we worked out a systematic formulation of failure under load as a homogeneous nucleation process, simulating the process via mean-field, Monte Carlo and molecular dynamics methods, for both model and semi-empirical interatomic potentials. We also developed a biased-random-walk description of microcrack propagation which incorporated for the first time the effects of surface reconstruction. Finally we extended multiple scattering analyses of composite and concrete materials to the limit of high crack density, allowing for new nondestructive evaluations of this important class of materials.

14. SUBJECT TERMS			15. NUMBER OF PAGES
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

PERFORMANCE PREDICTIONS FOR COMPOSITE MATERIALS

FINAL REPORT

Principal Investigators:

Professor William M. Gelbart
Professor Shechao Feng
Professor Howard Reiss
Professor Daniel Kivelson

December 31, 1993

U. S. ARMY RESEARCH OFFICE

CONTRACT NUMBER DAAL03-89-K-0144

Period of performance: 9/18/89 - 12/31/91

INSTITUTION:

Departments of Chemistry and Physics
University of California, Los Angeles
Los Angeles, CA 90024

APPROVED FOR PUBLIC RELEASE:
DISTRIBUTION UNLIMITED

FOREWORD:

In the report which follows we provide a concise statement of each of the six (6) individual projects carried out under Contract Number DAAL-03-89-K-0144, entitled "Performance Predictions for Composite Materials". The Principal Investigators (P.I.'s) and research students and postdoctoral assistants asssociated with each project are listed. We also supply for each of them a summary of the most important results which we obtained. The publications resulting from these investigations are cited, and twenty (15) copies of each are included with this report.

The scientific personnel participating in this contract work included

three postdoctoral assistants:
Dr. Zhen-Gang Wang
Dr. Robin Selinger
Dr. Leo Golubovic

two doctoral students:
Mr. Mark Sharlow
Mr. Hui-Lin Zhao

and

three visiting scientists:
Prof. Avinoam Ben-Shaul
Dr. Didier Sornette
Dr. Boris Spivak

Only the two doctoral students remain presently at UCLA, expecting to complete earn their PhD degrees during this coming year.

TECHNICAL REPORT -- Projects completed under
DARPA/ARMY CONTRACT DAAL-03-89-K-0144
(8/18/89 - 12/31/91)

1. Spin hamiltonian and elastic network models for treating the statistical thermodynamics of the failure of solids under stress.

This project involved a colloboration between two postdoctoral students, Dr. Robin Selinger and Dr. Zhen-Gang Wang, P.I. Professor William Gelbart, and a visitor, Professor Avinoam Ben-Shaul of the Hebrew University of Jerusalem. Here we formulated the first systematic statistical mechanical theory of the failure of solids under stress, by developing a complete analogy with the phenomenon of homogeneous nucleation in supersaturated vapors or undercooled liquids. More explicitly, the idea was to understand critical stresses and tensions as metastability limits for the system under external load. Correspondingly, the solid under stress is shown to be no longer in statistical thermodynamic equilibrium but rather to be only in a *metastable* state, from which the appearance of the *equilibrium* state (under load) -- broken solid -- will occur as soon as the *spinodal* is approached sufficiently closely for *nucleation* (of defects here) to occur at a physically interesting rate. Furthermore, increasing temperature is argued to play a significant effect in decreasing the critical loads which can be tolerated. This argument is then illustrated for two specific model systems, each describing the elastic solid under tension: an Ising-like collection of spins, and a network of breakable springs. Both mean-field solutions and numerical simulations establish the existence of a unique critical tensile force at which failure of the loaded systems occurs via a classical nucleation process. These results appeared in The Physical Review (A43, 4396 (1991)).

2. Molecular dynamics (atomistic computer simulation) description of the failure of model solids.

While several recent attempts have been advanced by others to describe solids under stress via atomistic modelling, e.g., Monte Carlo or molecular dynamics, none of these studies was performed within the systematic context of trying to establish general metastability limits for different failure modes of ideal systems at finite

temperature. Accordingly, a project along these latter lines was undertaken, enlisting the collobaration of (again Drs. Selinger and Wang, and Professor Gelbart, but this time also taking advantage of the computer modelling expertise of) Professor Uzi Landman of Georgia Tech. Specifically, we treated the well-known model system "Lennard-Jonesium", in two dimensions, subjecting it to successively larger tensile stresses at various temperatures and pressures, and solving numerically the effective (Lagrangian) equations of motion with help of periodic boundary conditions. In this way we were able to demonstrate explicitly the metastable nature of the less-than-critically-stressed solid: namely, imposing a small enough tensile force led to the system "pulling back" with an equal and opposite restoring force, essentially indefinitely. However, when the applied tension was within about 1% of a certain (perfectly reproducible) critical value, the restoring force was seen to drop to zero after a short time, indicating the failure of the (previously perfect) solid as it relieves stress by (developing holes and small-scale dislocation pairs as a prelude to) breaking into pieces. In addition, the role of thermal fluctuations was clearly established by observing a dramatic decrease (50%) in critical tension as the temperature is raised to, say, half the melting temperature. See our published account in The Physical Review (B44, 378 (1991)).

3. Statistical mechanical study of the interactions between thermal fluctuations and pre-existing defects in critically stressed solids.

Here, the project undertaken by Drs. Selinger and Wang and Professor Gelbart was intended to determine the extent to which pre-existing defects compete with increased temperature in lowering the threshold for failure of solids under external stress. The problem was treated first from the a quasi-analytic, mean-field, point of view, and then by means of large-scale Monte Carlo (computer) simulations. In these ways we succeeded in establishing the precise way in which defects lower the strength of an otherwise-ideal solid, investigating not only single-to-several-adjacent-site vacancies but also substitutional impurites. In all cases the key to understanding the (lowering of the applied stress) threshold to failure is the attainment of a critical *local* stress in the immediate region of the defect. (All of the relevant quantities are computed directly via purely microscopic/atomic expressions for the appropriate components of the anisotropic pressure tensor.) This critical local stress is shown to be an *intrinsic* property of the material, and direct

connections are made to the familiar *continuum* theory of stress concentration near crack tips. But now the role of temperature and thermal fluctuations are treated on the same footing as the pre-existing defects: see publication of our work in the Journal of Chemical Physics (95, 9128 (1991)).

4. Competition between failure and melting under stress in more realistic models of solids.

All of the work described above had been restricted largely to low temperatures where failure proceeded relatively straightforwardly as a *brittle* process. Also, our calculations were relevant to *two*-dimensional systems whose interaction potential was of the *model* (e.g., Lennard-Jones) type. In the final computer simulation study, then, carried out in collaboration between Dr. Selinger, Professor Gelbart, and a visitor Professor Ruth Lynden-Bell from Cambridge University (England), we investigated the properties of a *three*-dimensional solid whose interaction potential was of the semi-empirical, many-body, embedded-atom, type, and whose temperature was alternately allowed to be both very low with respect to T_{melt} *and comparable* to T_{melt}. Novel hybrid forms of Monte Carlo and molecular dynamics simulation methods are developed, allowing explicitly for arbitrary symmetry (e.g., cubic vs hexagonal, etc.) of the system. We found that, at low temperature, the solid (modelled here to be platinum), when subjected to tension, undergoes a phase transition to a more open crystalline structure before ultimately breaking via brittle fracture. At temperatures sufficiently close to T_{melt}, however, the solid relieves tensile stresses by *flowing* (melting) instead of breaking, demonstrating for the first time via a fully microscopic theory the nature of stress-induced melting. These results are presented in the Journal of Chemical Physics (98, 9808 (1993)).

5. Theoretical study of acoustical nondestructive evaluation of composite and concrete materials containing many cracks in the multiple scattering regime.

This project was carried out in a collaboration between P.I. Professor Shechao Feng and a visitor, Dr. Didier Sornette from the University of Nice (France). In this work we applied recently obtained understanding about correlations in multiple scattering to the problem of using ultrasonic waves to nondestructively detect the onset of *new* cracks in composite and concrete materials which

already contain a large number of cracks. In the regime where the acoustic wave undergoes multiple scattering as it travels through the sample, the outgoing intensity pattern is a random-looking speckle pattern which is normally thought to include no useful information about the system. But since the multiply scattered wave involves a *coherent* and therefore *correlated* process, one can view the observed speckle pattern as a kind of "fingerprint" of the positions of the cracks already present. Our work showed how the statistical average of the *change* in speckle pattern due to the addition of a crack can be computed: in this way we established how it is indeed possible, after averaging over a large number of frequencies, to locate the position of this newly formed crack. We believe our principle will be of use in extending for the first time acoustical nondestructive evaluations of cracks and other imperfections in composite materials *to the limit of high crack density.* Our work was published in the Journal of the Acoustical Society of America (90, 1742 (1991)).

6. Rate of microcrack healing and nucleation in solids under loading stress.

This project was pursued by Professor Feng in colloboration with a postdoctoral student, Dr. Leo Golubovic. We proposed here a phenomenological model for microcrack propagation in simple solids under a constant external stress. Specifically, we established the conditions under which the kinetics of crack nucleation processes should be qualitatively different from those occuring in simple metastable states such as supercooled liquids or supersaturated solutions. This difference is caused by irreversible processes such as surface diffusion and reconstruction which "denature" the faces of the microcrack. We argued in particular that such restructuring inhibits the healing of microcracks and thereby causes them to nucleate at rates much *faster* than those obtained from directly applying nucleation "laws" appropriate to metastable states in *fluid* systems, e.g., neat liquids and many-component solutions. The key idea is that the dynamics of growth/propagation need to be described by a *directed/biased* diffusion model, once the crack exceeds the atomic-scale dimensions implicitly assumed in our work on the *earlier* stages of defect formation in solids under stress. This project was published in the Physical Review (A43, 5223 (1991)).